Interacting Bosons at Finite Temperature: How Bogolubov Visited a Black Hole and Came Home Again

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Abstract

The structure of the thermal equilibrium state of a weakly interacting Bose gas is of current interest. We calculate the density matrix of that state in two ways. The most effective method, in terms of yielding a simple, explicit answer, is to construct a generating function within the traditional framework of quantum statistical mechanics. The alternative method, arguably more interesting, is to construct the thermal state as a vector state in an artificial system with twice as many degrees of freedom. It is well known that this construction has an actual physical realization in the quantum thermodynamics of black holes, where the added degrees of freedom correspond to the second sheet of the Kruskal manifold and the thermal vector state is a state of the Unruh or the Hartle–Hawking type. What is unusual about the present work is that the Bogolubov transformation used to construct the thermal state combines in a rather symmetrical way with Bogolubov's original transformation of the same form, used to implement the interaction of the nonideal gas in linear approximation. In addition to providing a density matrix, the method makes it possible to calculate efficiently certain expectation values directly in terms of the thermal vector state of the doubled system.

1 Introduction

The temperature of black holes, predicted and investigated by Jacob Bekenstein on the basis of classical thermodynamic and statistical reasoning [1, 2], is intimately related to the mixing of normal modes in quantum field theory. In the work of Hawking [3] (see also [4]) the disappearance of half the degrees of freedom of a field into the black hole was shown to be responsible for the entropy and temperature of the remaining degrees of freedom as an astrophysical black hole evaporates. Unruh [5] constructed radiating and (implicitly — cf. [6, 7]) equilibrium states of a quantum field on the maximal Kruskal extension ("eternal" black hole) in terms of coherent combinations of normal modes on the two sheets of the wormhole. The analytic continuation involved in the Unruh construction (which tells precisely how to combine positive-frequency modes on the physical sheet with negative-frequency modes on the unphysical sheet to create a state for the physical modes alone that is thermal at infinity) was soon recognized [8, 9, 10] to be an instance of the generic analyticity property of thermal states in a complex

time coordinate [11, 12]. Parker [13] showed that the well-known mixing of positive- and negative-frequency modes in cosmological models would give rise to a thermal spectrum of created particles under some (restricted but plausible) conditions. (In Parker's scenario the two members of a correlated pair are both physical, but they are effectively rendered decoherent by spatial separation.)

Israel [14] and Sewell [9] recognized Unruh's construction as a physical realization of a more abstract construction already known in quantum statistical mechanics [15, 12, 16]. In the latter, a fictitious copy of the physical system is introduced and its modes are mixed with the physical modes to produce a thermal state of the latter. (We review the details in the next section, for the case of a free boson system.) In Unruh's scenario the second set of modes is not fictitious. At worst, it resides on the second sheet of the Kruskal wormhole; for a uniformly accelerating observer in flat space-time or an inertial observer in de Sitter space, it belongs to the part of ordinary space-time beyond the observer's horizon [5, 17, 18, 7].

Black-hole temperature and cosmological particle production are effects in linear (noninteracting) quantum field theory in curved space-time that amount mathematically to linear mixing of creation and annihilation operators in a way that preserves their canonical commutation (or anticommutation) relations. Typically one set of operators defines a Fock-space structure so that the state under investigation is the corresponding vacuum, or no-quantum, state, while the other set of operators corresponds directly to physical observations. This type of construction (which pervades [3, 4, 5, 7, 13]) is called a *Bogolubov transformation*.

It is important to note that originally the Bogolubov transformation had nothing to do with either gravitational physics or temperature. N. N. Bogolubov [19, 20] introduced it to find the *ground* state of a system of *interacting* massive bosons, such as atoms. More precisely, the original application was to ultracold helium, for which it turned out not to be quite adequate; but nevertheless, it has become a central tool in condensed-matter physics. In recent years, the necessity of a more detailed understanding of ultracold gases of weakly interacting bosons brought about many new applications of Bogolubov's formalism in physical contexts where the underlying approximations are quite reliable. A recent article of Zagrebnov and Bru [21] discusses these approximations, provides additional references to Bogolubov's pioneering work, and reviews the current mathematical status of the theory.

Our exposition of Bogolubov's theory follows that of Kocharovsky et al.

[22]. Under the assumption of a two-body interaction, the Hamiltonian is of the form

$$H = \sum_{\mathbf{k}} \frac{\hbar^2 \mathbf{k}^2}{2M} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \sum_{\mathbf{k}_j} U_{\mathbf{k}_1\mathbf{k}_2,\mathbf{k}_3\mathbf{k}_4} a_{\mathbf{k}_1}^\dagger a_{\mathbf{k}_2}^\dagger a_{\mathbf{k}_3} a_{\mathbf{k}_4} \,. \tag{1}$$

If the interaction U is sufficiently weak, most of the atoms will remain in the ground mode of the noninteracting theory ("Bose condensate"), and the excitations out of that mode can be treated to good approximation by a linearization of H. One introduces new operators

$$\beta_0 = \frac{a_0}{\sqrt{a_0^\dagger a_0 + 1}}\,, \qquad \beta_{\mathbf{k}} = \beta_0^\dagger a_{\mathbf{k}} \quad \text{for } \mathbf{k} \neq 0. \tag{2}$$

The operators with $\mathbf{k} \neq 0$ satisfy the canonical relations $[\beta_{\mathbf{k}}, \beta_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k},\mathbf{k}'}$, and one can assume that terms in H containing more than two of them are negligible, so that H is approximately of the form

$$H_B = E_0 + \sum_{\mathbf{k}\neq 0} V_{\mathbf{k}} \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} + \sum_{\mathbf{k}\neq 0} (W_{\mathbf{k}} \beta_{\mathbf{k}} \beta_{-\mathbf{k}} + \text{H.c.}), \tag{3}$$

with coefficients independent of the sign of $\mathbf{k}$. (Conservation of momentum and of parity have been assumed here. At the next step we assume positivity of the energy.) It is well known how to "diagonalize" such a quadratic Hamiltonian by a Bogolubov transformation:

$$\beta_{\mathbf{k}} = u_{\mathbf{k}} b_{\mathbf{k}} + v_{\mathbf{k}} b_{-\mathbf{k}}^\dagger, \qquad |u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 = 1; \tag{4}$$

$$H_B = E_0 + \sum_{\mathbf{k}\neq 0} \epsilon_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}. \tag{5}$$

(All the undefined quantities in (3), (4), (5) can be calculated from the U and M in (1); the details are not important here.) The dynamics of the system in the b variables is now trivial; for physical interpretation one returns to the β variables, for example, to see the structure of the physical ground state in terms of real atoms.

In the wake of the recent experimental observations of Bose condensation of atoms [23], interest in the type of problem originally investigated by Bogolubov has intensified. Methods have been invented to measure directly the (magnitudes of the) amplitudes $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ in (4) in a Bose–Einstein condensate [24]. In [22] the (weakly) interacting Bose gas was studied at (low but) finite temperature; formulas were found for the characteristic function

(Fourier-transformed probability distribution) of the total number of atoms in a pair of modes, $\beta_{\mathbf{k}}^\dagger\beta_{\mathbf{k}} + \beta_{-\mathbf{k}}^\dagger\beta_{-\mathbf{k}}$, and some related statistical quantities (the generating cumulants). In [22] the interaction was treated as above, and the temperature was treated by constructing the statistical operator (density matrix) for each mode in the traditional, direct way:

$$\rho_{\mathbf{k}} = (1 - e^{-\epsilon_{\mathbf{k}}/T})e^{-\epsilon_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}/T}. \tag{6}$$

(Note that it is the dressed (b) quanta that appear in (6), because the Hamiltonian is (5), but it is the bare (β) quanta whose statistics are being studied.) The formulas of [22] are expressed in terms of a quantity

$$z(A_{\mathbf{k}}) = \frac{A_{\mathbf{k}} - e^{\epsilon_{\mathbf{k}}/T}}{A_{\mathbf{k}} e^{\epsilon_{\mathbf{k}}/T} - 1} \tag{7}$$

and $z(-A_{\mathbf{k}})$, where $A_{\mathbf{k}} = v_{\mathbf{k}}/u_{\mathbf{k}}$ is the parameter defining the Bogolubov transformation (4).

We recall that when $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are real-valued, which one may assure by choosing the phases of the modes properly, it is customary to write the coefficients in (4) as

$$u_{\mathbf{k}} = \cosh\theta_{\mathbf{k}}, \quad v_{\mathbf{k}} = \sinh\theta_{\mathbf{k}}; \qquad A_{\mathbf{k}} = \tanh\theta_{\mathbf{k}}\,. \tag{8}$$

(Henceforth we drop the subscript $\mathbf{k}$ whenever no ambiguity results.) Then θ is an additive quantity precisely analogous to the rapidity parameter of a Lorentz transformation; that is, the result of successively applying two Bogolubov transformations is the Bogolubov transformation corresponding to the sum of the respective θs. Now (7) superficially resembles the addition formula for the hyperbolic tangent function,

$$\tanh(x \pm y) = \frac{\tanh x \pm \tanh y}{1 \pm \tanh x \tanh y}\,. \tag{9}$$

This suggests that the results of [22] can be better understood, and perhaps more easily derived, in terms of the composition of the transformation of the original Bogolubov type (implementing the interaction) with a Bogolubov transformation of the Unruh type to implement the thermalization. Unfortunately, there are three things wrong with this naive idea. First, $e^{\epsilon/T}$ is greater than unity, and hence cannot be a hyperbolic tangent. Fortunately, that problem is instantly solved by rewriting (7) as

$$-\frac{1}{z(A)} = \frac{Ae^{\epsilon/T} - 1}{e^{\epsilon/T} - A} = \frac{A - e^{-\epsilon/T}}{1 - Ae^{-\epsilon/T}}\,, \tag{10}$$

which really does have the form (9). Second [see (20)], the correct Bogolubov parameter in the Unruh (more properly, the Araki–Woods–Takahashi–Umezawa) construction is $e^{-\epsilon/2T}$, not $e^{-\epsilon/T}$. And third, the two Bogolubov transformations are about "different axes" in a space of dimension greater than 2, so there is no reason to expect them to compose in such a simple way.

The present authors [25] rederived (and generalized) the results of [22] in a simpler way, without, however, elucidating any connection with the thermal Bogolubov construction. Here we present (in Secs. 2 and 4) a direct assault on the problem by the thermal Bogolubov method. Inevitably, the treatment displays a certain "hidden symmetry" between the parameters

$$\theta = \tanh^{-1} A \quad \text{and} \quad \phi = \tanh^{-1} e^{-\epsilon/2T}. \tag{11}$$

Equally inevitably, this symmetry is largely destroyed in the final formula for the density matrix, since to get it one must trace over the fictitious modes of the thermal construction but does not trace over any of the physical modes involved in the Bogolubov dressing transformation (see Sec. 3). However, the symmetry is restored when one takes the expectation value of an observable that involves only *one* physical traveling-wave mode. In fact, the moments and cumulants associated with the number operators for one or two modes can be most easily calculated directly from the Araki–Takahashi–Unruh pure state vector, rather than from the density matrix (Sec. 5). In Sec. 6, to obtain a simpler form for the density-matrix elements (generalizing [25]) we employ a different method, based on generating functions.

2 Main calculation

The analysis proceeds in seven steps.

2.1 Reduction to standing-wave modes

Introduce (for each pair $\pm\mathbf{k}$)

$$b_c = \frac{b_{\mathbf{k}} + b_{-\mathbf{k}}}{\sqrt{2}}\,, \quad b_s = \frac{b_{\mathbf{k}} - b_{-\mathbf{k}}}{\sqrt{2}}\,, \tag{12}$$

so that

$$b_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} + b_{-\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{x}} = \sqrt{2}[b_c \cos{(\mathbf{k}\cdot\mathbf{x})} + i b_s \sin{(\mathbf{k}\cdot\mathbf{x})}]\,,$$

$$b^\dagger_{\mathbf{k}} b_{\mathbf{k}} + b^\dagger_{-\mathbf{k}} b_{-\mathbf{k}} = b^\dagger_c b_c + b^\dagger_s b_s \,, \tag{13}$$

and these operators and their adjoints satisfy the canonical commutation relations. Henceforth we concentrate largely on the cosine modes and often omit the subscript c.

2.2 Dressing by the interaction

The Bogolubov transformation (4) and (8) is chosen to convert (3) into (5). The inverse of such a transformation is the same except for the sign of θ, A, and v. The transformation thereby induced on the cosine modes is

$$\beta = \cosh\theta\, b + \sinh\theta\, b^\dagger; \qquad b = \cosh\theta\, \beta - \sinh\theta\, \beta^\dagger; \qquad \theta = \tanh^{-1} A. \tag{14}$$

The transformation of the sine modes has the opposite sense:

$$\beta_s = \cosh\theta\, b_s - \sinh\theta\, b^\dagger_s; \qquad b_s = \cosh\theta\, \beta_s + \sinh\theta\, \beta^\dagger_s. \tag{15}$$

(This strange sign is an artifact of our phase convention in (12); it could be avoided at the cost of unnecessary imaginary numbers elsewhere.)

Recall that β annihilates bare quasiparticles, here interpreted as excited physical atoms, while b annihilates dressed quanta, so that the eigenstates of energy are eigenstates of the number operator $b^\dagger b$. If $|0)$ is the ground state: $b|0) = 0$, and $|n\rangle$ is the state of n physical atoms: $\beta^\dagger\beta|n\rangle = n|n\rangle$, then

$$|0) = \frac{1}{\sqrt{\cosh\theta}} \sum_{j=0}^{\infty} A^j \sqrt{\frac{(2j-1)!!}{(2j)!!}}\, |2j\rangle \qquad (A = \tanh\theta). \tag{16}$$

It is instructive to review the proof of (16): Write $|0)$ as $N\sum_{n=0}^{\infty} c_n|n\rangle$ with $c_0 = 1$. Impose the condition that $(\cosh\theta\,\beta - \sinh\theta\,\beta^\dagger)|0) = 0$ to obtain the recursion $c_{n+1} = \sqrt{\frac{n}{n+1}}\tanh\theta\, c_{n-1}$. It follows that $c_n = 0$ for odd n and $c_{2j} = A^j\sqrt{(2j-1)!!/(2j)!!}$ (where $n!! = n(n-2)\cdots$). Impose the requirement that $(0|0) = 1$ and observe that

$$\frac{1}{\sqrt{1-x}} = \sum_{j=0}^{\infty} x^j\, \frac{(2j-1)!!}{(2j)!!} \tag{17}$$

to conclude that $N^2 = \sqrt{1-\tanh^2\theta} = (\cosh\theta)^{-1}$.

2.3 Thermal dressing

The thermal Bogolubov construction must be applied to the energy eigenstates, regardless of whether there is an interaction. So (working with one mode at a time) we start from the number eigenstates satisfying

$$b|0) = 0 \quad \text{and} \quad b^\dagger b|n) = n|n)\,. \tag{18}$$

Now introduce a fictitious mode "on the other side of the world" with corresponding operators $\overline{b}$ and $\overline{b}^\dagger$; we work in a doubled Fock space with basis vectors satisfying

$$b|0,0) = 0\,, \quad \overline{b}|0,0) = 0\,; \qquad b^\dagger b|n,m) = n|n,m)\,, \quad \overline{b}^\dagger\overline{b}|n,m) = m|n,m)\,. \tag{19}$$

The thermal Bogolubov transformation is [16, 5]

$$c = \cosh\phi\, b - \sinh\phi\, \overline{b}^\dagger, \quad \overline{c} = \cosh\phi\, \overline{b} - \sinh\phi\, b^\dagger; \qquad e^{-\epsilon/2T} = \tanh\phi, \tag{20}$$

with inverse $b = \cosh\phi\, c + \sinh\phi\, \overline{c}^\dagger$, $\overline{b} = \cosh\phi\, \overline{c} + \sinh\phi\, c^\dagger$.

Let $|0,0\}$ be the state with no c and $\overline{c}$ quanta: $c|0,0\} = 0 = \overline{c}|0,0\}$. Then

$$|0,0\} = \frac{1}{\cosh\phi}\sum_{n=0}^{\infty} \tanh^n\phi\, |n,n) = (1 - e^{-\epsilon/T})^{1/2}\sum_{n=0}^{\infty} e^{-n\epsilon/2t}|n,n). \tag{21}$$

The proof is parallel to that of (16) and slightly simpler, because the alternating-factorial and consequent square-root functions do not arise.

The statistical (density) operator for the whole system (of one real and one fictitious mode) is

$$|0,0\}\{0,0| = (1 - e^{-\epsilon/T})\sum_{n,m=0}^{\infty} e^{-(n+m)\epsilon/2T}|n,n)(m,m|. \tag{22}$$

The statistical operator for the physical mode alone is obtained by tracing over the states of the unphysical mode:

$$\rho = (1 - e^{-\epsilon/T})\sum_{n=0}^{\infty} e^{-n\epsilon/T}|n)(n|. \tag{23}$$

By design, ρ is precisely [cf. (6)] the thermal ensemble at temperature T! This is the generic Araki–Takahashi–Unruh construction, in the setting of our particular problem.

The foregoing notation is appropriate for the cosine modes. For the sine modes, we choose to change the sign of ϕ in (20). This convention corresponds to the natural, momentum-conserving Bogolubov transformation (43) on the original traveling-wave modes (where $b_{\mathbf{k}}$ mixes with $b^\dagger_{-\mathbf{k}}$, not $b^\dagger_{\mathbf{k}}$), which is mandatory in an Unruh-type situation but arbitrary when the barred modes are completely fictitious. The sign cancels in the final reduced density matrix, (23).

2.4 Diagonalization of the composite transformation

We now combine (14) and (20) to express the bare modes in terms of the doubly dressed modes:

$$\begin{pmatrix} \beta \\ \beta^\dagger \\ \overline{\beta} \\ \overline{\beta}^\dagger \end{pmatrix} = \begin{pmatrix} up & vp & vq & uq \\ vp & up & uq & vq \\ vq & uq & up & vp \\ uq & vq & vp & up \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \\ \overline{c} \\ \overline{c}^\dagger \end{pmatrix}. \tag{24}$$

(Here $p = \cosh\phi$, $q = \sinh\phi$, and $\overline{\beta}$ is related to $\overline{b}$ just as β is to b.) Introduce

$$\Omega = \theta + \phi, \quad \Psi = \theta - \phi, \tag{25}$$

and

$$G = \frac{\beta + \overline{\beta}}{\sqrt{2}}, \quad H = \frac{\beta - \overline{\beta}}{\sqrt{2}}, \qquad \gamma = \frac{c + \overline{c}}{\sqrt{2}}, \quad \delta = \frac{c - \overline{c}}{\sqrt{2}}. \tag{26}$$

Then a short calculation shows that

$$G = \cosh\Omega\,\gamma + \sinh\Omega\,\gamma^\dagger, \quad H = \cosh\Psi\,\delta + \sinh\Psi\,\delta^\dagger. \tag{27}$$

That is, (24) decouples into two elementary Bogolubov transformations! Moreover, the idea that (9) should be playing a role is vindicated by (25).

2.5 Construction of the thermal state with interaction

Note that the state annihilated by γ and δ is the same as $|0,0\}$, the one annihilated by c and $\overline{c}$; after tracing over the barred mode, it will give us the thermal state we want. But to interpret that state we need to express it in terms of the $\beta^\dagger\beta$ number observable.

The first step is to construct $|0,0\}$ within the (G,H) Fock space. This is done by applying the mathematics of (16) to the two transformations (27) independently. We need to define yet another basis:

$$G^\dagger G|J,L] = J|J,L], \quad H^\dagger H|J,L] = L|J,L]. \tag{28}$$

Then

$$|0,0\} = \frac{1}{\sqrt{\cosh\Omega\cosh\Psi}} \sum_{j,l=0}^{\infty} \tanh^j\Omega\tanh^l\Psi \sqrt{\frac{(2j-1)!!\,(2l-1)!!}{(2j)!!\,(2l)!!}}\,|2j,2l]. \tag{29}$$

The basis of physical interest is defined by

$$\beta^\dagger\beta|n,m\rangle = n|n,m\rangle, \quad \overline{\beta}^\dagger\overline{\beta}|n,m\rangle = m|n,m\rangle. \tag{30}$$

In view of (26), the connection between $|J,L]$ and $|n,m\rangle$ is just a unitary transformation, introducing no further pair creation. (Nevertheless, it is the source of most of the combinatorial complexity of our result.) One has

$$\begin{aligned}
|2j,2l] &= \frac{1}{\sqrt{(2j)!}}(G^\dagger)^{2j}\frac{1}{\sqrt{(2l)!}}(H^\dagger)^{2l}|0,0] \\
&= \frac{1}{2^{j+l}\sqrt{(2j)!\,(2l)!}} \sum_{\kappa=0}^{2j}\sum_{\lambda=0}^{2l} \binom{2j}{\kappa}\binom{2l}{\lambda}(-1)^\lambda \\
&\quad \times (\beta^\dagger)^{2j-\kappa+2l-\lambda}(\overline{\beta}^\dagger)^{\kappa+\lambda}|0,0\rangle \\
&= \frac{1}{2^{j+l}}\sum_{\kappa,\lambda}\frac{(-1)^\lambda\sqrt{(2j)!\,(2l)!}}{\kappa!\,(2j-\kappa)!\,\lambda!\,(2l-\lambda)!} \\
&\quad \times \sqrt{(2j+2l-\kappa-\lambda)!\,(\kappa+\lambda)!}|2j+2l-\kappa-\lambda,\kappa+\lambda\rangle.
\end{aligned} \tag{31}$$

Introduce $m = \kappa+\lambda$ and define

$$Q(m,j,l) = \sum_{\lambda=\max(0,m-2j)}^{\min(m,2l)} \frac{(-1)^\lambda}{\lambda!\,(2l-\lambda)!\,(m-\lambda)!\,(2j-m+\lambda)!}\,. \tag{32}$$

Then

$$|2j,2l] = \frac{\sqrt{(2j)!\,(2l)!}}{2^{j+l}} \sum_{m=0}^{2j+2l} \sqrt{(2j+2l-m)!\,m!}\,Q(m,j,l)\,|2j+2l-m,m\rangle. \tag{33}$$

Substituting (33) into (29) and simplifying, one obtains (for a cosine mode)

$$
\begin{aligned}
|0,0\} = {} & \frac{1}{\sqrt{\cosh\Omega\cosh\Psi}} \sum_{\substack{n,m=0\\ n+m \text{ even}}}^{\infty} |n,m\rangle\sqrt{n!\,m!} \\
& \times \sum_{l=0}^{p} \tanh^{p-l}\Omega\, \tanh^{l}\Psi\, \frac{(2l)!\,(2p-2l)!}{4^p\, l!\,(p-l)!}\, Q(m,p-l,l), \qquad (34)
\end{aligned}
$$

where $p = \frac{1}{2}(n+m)$. For a sine mode, a factor $(-1)^p$ should be inserted.

2.6 Evaluation of Q

First note that whenever λ is outside the range specified in (32), the summand is 0 because at least one of the denominator factors is at a pole of the gamma function. Therefore, one may extend the summation over $-\infty < \lambda < \infty$, and it is not necessary to write the limits at all [26].

Now define

$$
P(a,c,m) = 2^{-m} \sum_{\lambda} (-1)^{\lambda} \binom{c-a}{m-\lambda}\binom{a}{\lambda}. \qquad (35)
$$

Then, on the one hand,

$$
P(a,c,m) = P_m^{(c-a-m,a-m)}(0), \qquad (36)
$$

where $P_m^{(\alpha,\beta)}(x)$ is a Jacobi polynomial [27]. (This special value of the Jacobi polynomial apparently cannot be reduced to anything simpler; the very systematic software associated with [28] identifies it as a certain hypergeometric function (also in [27]) but nothing less.) On the other hand, we have

$$
4^{-p}\,(2l)!\,(2p-2l)!\,Q(m,p-l,l) = 2^{-n} P(2l,2p,m) \qquad (p = \tfrac{1}{2}(n+m)). \quad (37)
$$

In this notation (34) becomes

$$
\begin{aligned}
|0,0\} = {} & \frac{1}{\sqrt{\cosh\Omega\cosh\Psi}} \sum_{\substack{n,m=0\\ n+m \text{ even}}}^{\infty} |n,m\rangle\sqrt{n!\,m!} \\
& \times \sum_{l=0}^{p} \tanh^{p-l}\Omega\, \tanh^{l}\Psi\, \frac{1}{2^n\, l!\,(p-l)!}\, P(2l,2p,m). \qquad (38)
\end{aligned}
$$

2.7 The density matrix

The density matrix $\rho_{nn'} = \langle n|\rho|n'\rangle$ for a cosine mode is obtained by tracing $|0,0\}\{0,0|$ over the states of the fictitious partner mode. That is, in a linear combination of objects $|n,m\rangle\langle n',m'|$ one must set $m'=m$ and sum over m. Since $n-m$ and $n'-m'$ are constrained to be even, the result is 0 unless $n-n'$ is even. One gets

$$\rho_{nn'} = 0 \quad \text{if } n-n' \text{ is odd}, \tag{39}$$

$$\begin{aligned} \rho_{nn'} &= \frac{1}{\cosh\Omega\cosh\Psi}\,\frac{\sqrt{n!\,n'!}}{2^{n+n'}} \sum_{\substack{m=0\\ n-m \text{ even}}}^{\infty} m! \\ &\quad \times \sum_{l=0}^{p}\sum_{l'=0}^{p'} \frac{P(2l,2p,m)P(2l',2p',m)}{l!\,l'!\,(p-l)!\,(p'-l')!}\tanh^{p+p'-l-l'}\Omega\,\tanh^{l+l'}\Psi, \\ &\quad p=\frac{n+m}{2},\quad p'=\frac{n'+m}{2},\quad n-n' \text{ even}. \end{aligned} \tag{40}$$

(The limits on the l and l' summations are superfluous, for the same reason explained earlier for λ.)

The density matrix for a sine mode is the same except for a factor $(-1)^{(n-n')/2}$. The density matrix for the entire atomic system is the tensor product of all the density matrices for the individual modes. (Recall that the latter depend on $|\mathbf{k}|$ through Ω and Ψ.)

3 Symmetries (or not)

The *Jacobi number* (35) has these symmetries:

$$\begin{gathered} P(c-a,c,m) = (-1)^m P(a,c,m)\,; \\ 2^m P(a,c,m) = (-1)^a 2^n P(a,c,n) \quad \text{if } n+m=c. \end{gathered} \tag{41}$$

The first of these (with $c=2p$, $a=2l$) expresses the essential invariance of our formulas when a summation index l is changed to $p-l$, hence when Ω interchanged with Ψ. The second (with a even) expresses the symmetry of $|0,0\}$ in the real and fictitious modes.

It is time to contemplate the meaning of Ω and Ψ in terms of the basic parameters of our problem, A and ϵ/T. From the definitions we have

$$\tanh\Omega = \frac{A+e^{-\epsilon/2T}}{1+Ae^{-\epsilon/2T}}\,, \quad \tanh\Psi = \frac{A-e^{-\epsilon/2T}}{1-Ae^{-\epsilon/2T}}\,. \tag{42}$$

These bear tantalizing resemblances to $\frac{1}{z(-A)}$ and $-\frac{1}{z(A)}$ as expressed through (10), but the factor of 2 with the temperature is ineradicable.

Now observe the behavior of the density matrix (40) under elementary operations on the parameters:

- Interchanging Ω and Ψ (i.e., changing the sign of ϕ) leaves ρ invariant. Since this operation amounts to replacing $e^{-\epsilon/2T}$ by a negative number, it may appear unphysical. However, as previously remarked in connection with the sine modes, it really represents just an arbitrariness in the definition of the fictitious modes.

- Changing the signs of both Ω and Ψ is equivalent to changing the signs of both θ and ϕ. Its effect on $\rho_{nn'}$ is an overall factor $(-1)^{(n-n')/2}$. This is precisely the distinction between cosine and sine modes.

- Interchanging θ and ϕ is equivalent to changing the sign of Ψ. Its effect on ρ is substantive: Each term in the summand is multiplied by $(-1)^{l+l'}$. Thus (of course) the final formulas of the theory are *not* all symmetric under interchange of an interaction parameter with a temperature parameter, despite the intriguing symmetries in the formalism. (We shall see later, however, that some formulas *are* symmetric.)

The other 4 nontrivial elements of the group generated by these operations add no additional insight.

4 A pair of modes

At the cost of dealing with twice as many indices, one can work directly with the original traveling-wave modes, skipping step (12). Some of the intermediate results are useful, so we summarize the calculation here.

Define a momentum-conserving thermal Bogolubov transformation

$$b_{\mathbf{k}} = p_{\mathbf{k}} c_{\mathbf{k}} + q_{\mathbf{k}} \overline{c}^{\dagger}_{-\mathbf{k}}\,, \quad \overline{b}_{\mathbf{k}} = p_{\mathbf{k}} \overline{c}_{\mathbf{k}} + q_{\mathbf{k}} c^{\dagger}_{-\mathbf{k}} \tag{43}$$

equivalent to (20) and its b_s counterpart. When (43) is combined with (4) and its barred counterpart, one obtains two 4×4 systems of precisely the form (24), except that all the creation operators have the opposite sign of $\mathbf{k}$ from the annihilation operators they mix with. So one can define operators as in (26), with subscripts $\pm$, and get

$$G_{\pm} = \cosh\Omega\,\gamma_{\pm} + \sinh\Omega\,\gamma^{\dagger}_{\mp}\,, \quad H_{\pm} = \cosh\Psi\,\delta_{\pm} + \sinh\Psi\,\delta^{\dagger}_{\mp}\,. \tag{44}$$

By the same methods as before, one finds that the analog of (29) is

$$|0,0,0,0\} = \frac{1}{\cosh\Omega\,\cosh\Psi}\sum_{j,l=0}^{\infty}\tanh^j\Omega\tanh^l\Psi|j,j]\otimes|l,l], \tag{45}$$

where $|0,0,0,0\}$ is annihilated by $\gamma_\pm$ and $\delta_\pm$, and

$$\begin{aligned} G_+^\dagger G_+|j,\tilde{\jmath}] &= j|j,\tilde{\jmath}], \quad H_+^\dagger H_+|l,\tilde{l}] = l|l,\tilde{l}], \\ G_-^\dagger G_-|j,\tilde{\jmath}] &= \tilde{\jmath}|j,\tilde{\jmath}], \quad H_-^\dagger H_-|l,\tilde{l}] = \tilde{l}|l,\tilde{l}]. \end{aligned} \tag{46}$$

Note that in (45) the occupation numbers may be either even or odd, but the number of G_+ quanta is always the same as the number of G_- quanta, and similarly for H. The analog of (45) for standing waves is the tensor product of (29) for the cosine mode with its partner for the sine mode; in that case, all occupation numbers must be even, but there is no constraint relating those for c quanta to those for s quanta.

Let $\rho_{n\tilde{n},n'\tilde{n}'}$ be the matrix element of the statistical operator between the state $\langle n\tilde{n}|$ with n (physical) β_+ quanta and $\tilde{n}$ β_- quanta and another such state $|n'\tilde{n}'\rangle$. A long calculation parallel to that leading to (40) yields

$$\rho_{n\tilde{n}n'\tilde{n}'} = 0 \quad \text{if } n-\tilde{n} \neq n'-\tilde{n}', \tag{47}$$

and otherwise

$$\begin{aligned} \rho_{n\tilde{n}n'\tilde{n}'} = {} & \frac{1}{\cosh^2\Omega\,\cosh^2\Psi}\sum_{m=0}^{\infty}\sum_{l=0}^{p}\sum_{l'=0}^{p'}\frac{\sqrt{n!\,\tilde{n}!\,n'!\,\tilde{n}'!}\,m!\,\tilde{m}!}{2^{p+p'-2m-2\tilde{m}}\,l!\,l'!\,(p-l)!\,(p'-l')!} \\ & \times P(l,p,m)P(l,p,\tilde{m})P(l',p',m)P(l',p',\tilde{m}) \\ & \times \tanh^{p+p'-l-l'}\Omega\,\tanh^{l+l'}\Psi, \\ & \tilde{m} = n+m-\tilde{n}, \quad p = n+m, \quad p' = n'+m. \end{aligned} \tag{48}$$

A corollary of the momentum conservation constraint (47) is that $n+\tilde{n}$ has the same parity as $n'+\tilde{n}'$ in any nonvanishing matrix element; this is necessary for consistency with (39) and with the general principle that Bogolubov transformations “create” quanta only in pairs.

5 Number observables

Henceforth it is convenient to write formulas in terms of

$$A = \tanh\theta \quad \text{and} \quad B = \tanh\phi = e^{-\epsilon/2T}. \tag{49}$$

Along with (42) we have (noting that $|AB| < 1$)

$$\cosh\Omega = \frac{1+AB}{\sqrt{(1-A^2)(1-B^2)}}\,, \quad \sinh\Omega = \frac{A+B}{\sqrt{(1-A^2)(1-B^2)}}\,,$$
$$\cosh\Psi = \frac{1-AB}{\sqrt{(1-A^2)(1-B^2)}}\,, \quad \sinh\Psi = \frac{A-B}{\sqrt{(1-A^2)(1-B^2)}}\,. \tag{50}$$

Our formalism provides two ways to calculate the expectation value of an operator. One may use the density matrix, (40) or (48). Alternatively, one can express the operator in terms of the operators G and H and their adjoints and take its matrix element in the pure state vector (29) or (45). For some observables the second method is much easier and also displays the $\theta \leftrightarrow \phi$ (or $A \leftrightarrow B$) symmetry to the maximal extent.

Consider a fixed mode pair $\pm\mathbf{k}$. Recall that all our creation and annihilation operators carry subscripts c, s, $+$, or $-$; we routinely omit not only any reference to the vector $\mathbf{k}$ but also the subscript (especially c or $+$), when no ambiguity results. When the sine mode is involved, the correct state vector is the product of (29) with its sine partner, whose formula is the same as (29) except for a factor $(-1)^{j+l}$ in the summand. For any mode type there is a number operator

$$n = \beta^\dagger\beta = \frac{1}{\sqrt{2}}(G^\dagger + H^\dagger)\frac{1}{\sqrt{2}}(G+H) = \frac{1}{2}(G^\dagger G + H^\dagger H + G^\dagger H + H^\dagger G). \tag{51}$$

5.1 The mean number

First consider $\langle n_+\rangle$ or $\langle n_-\rangle$. From (45) we see that only $G^\dagger G$ and $H^\dagger H$ contribute to $\langle n\rangle = \{0,0,0,0|n|0,0,0,0\}$, because the other two terms in (51) destroy the equality of the $+$ and $-$ occupation numbers. Using the first of

$$\sum_{j=0}^{\infty} jx^j = \frac{x}{(1-x)^2}\,, \quad \sum_{j=0}^{\infty} jx^j\,\frac{(2j-1)!!}{(2j)!!} = \frac{x}{2}(1-x)^{-3/2}, \tag{52}$$

along with (50), one calculates

$$\langle n\rangle = \frac{A^2+B^2}{(1-A^2)(1-B^2)}\,. \tag{53}$$

After chasing through several layers of definitions, one sees that (53) ought to coincide with (each term of) equation (72) of [22], and it does. Incidentally, (72) is one of very few formulas in [22] that are (even implicitly) symmetric in A and B. But it is now clear why it, and *any expectation value that concerns only one traveling-wave mode*, must have that symmetry: The thermal Bogolubov transformation (4) connecting that mode to one of the fictitious barred modes has the same algebraic form as the transformation (43) connecting that mode to another of the physical modes. When the expectation value is calculated, *all* other modes are effectively traced over, so there is nothing to distinguish the fictitious partner mode, with mixing constant B, from the physical one, with mixing constant A.

This argument does not apply to standing waves, because the transformation (14)–(15) does not have the same form as (43); in fact, we shall soon see that the conclusion does not hold for such modes. Nevertheless, a calculation based on (29) shows that

$$\langle n_c \rangle = \langle n_s \rangle = \langle n \rangle. \tag{54}$$

In this case the second of formulas (52) is used, and again the $G^\dagger H$ and $H^\dagger G$ terms in (51) do not contribute, but this time for a different reason: they produce occupation numbers of odd parity, which do not occur in $\{0, 0|$.

5.2 The second moment

The operator n^2 is

$$n^2 = \tfrac{1}{4}(O_R + O_P + O_I), \tag{55}$$

where the terms

$$O_R = (G^\dagger G)^2 + (H^\dagger H)^2 + 4G^\dagger G H^\dagger H + G^\dagger G + H^\dagger H \tag{56}$$

are *relevant*, the terms

$$O_P = (G^\dagger)^2 H^2 + (H^\dagger)^2 G^2 \tag{57}$$

are *partially relevant*, and the terms

$$O_I = 2[(G^\dagger)^2 G H + (H^\dagger)^2 H G + G^\dagger G^2 H^\dagger + H^\dagger H^2 G^\dagger + G^\dagger H + H^\dagger G] \tag{58}$$

are *irrelevant* because they contribute nothing to $\langle n^2 \rangle$. The partially relevant terms conserve parity but not momentum, so they contribute in the context of (29) but not (45).

For $\langle n_+^2\rangle$ or $\langle n_-^2\rangle$ a calculation like that of $\langle n\rangle$ leads to a formula that can be abbreviated as

$$\langle n^2\rangle = 2\langle n\rangle^2 + \langle n\rangle. \tag{59}$$

Since $\langle (n-\langle n\rangle)^2\rangle = \langle n^2\rangle - \langle n\rangle^2$, it follows that the second moment of the number distribution is

$$\langle (n-\langle n\rangle)^2\rangle = \langle n\rangle^2 + \langle n\rangle. \tag{60}$$

Again, these quantities are symmetric in A and B.

A parallel calculation yields

$$\langle n_c^2\rangle = \langle n_s^2\rangle = \frac{(1+B^2)[A^4+B^2+2A^2(1+B^2)]}{(1-A^2)^2(1-B^2)^2}\,. \tag{61}$$

Here the symmetry between A and B is destroyed by the contribution of the partially relevant terms.

5.3 The second cumulant

Kocharovsky et al. [22] do not give a formula for $\langle n^2\rangle$; the closest point of comparison is the *generating cumulant* $\tilde\kappa_2$. One case of their formula (71) is, after reexpression in terms of A and B rather than $z(A)$ and $z(-A)$,

$$\begin{aligned}\tilde\kappa_2 &= \frac{A^2B^4+A^4+4A^2B^2+B^4+A^2}{(1-A^2)^2(1-B^2)^2} \\ &= \langle n^2\rangle + \frac{A^2(B^2+1)^2}{(1-A^2)^2(1-B^2)^2}\,.\end{aligned} \tag{62}$$

Note that the second term is not symmetric in A and B.

This cumulant refers to a *pair* of modes, $\pm\mathbf{k}$. Its definition is

$$\begin{aligned}\tilde\kappa_2 &= \tfrac{1}{2}[\langle (n_+ + n_- - 2\langle n\rangle)^2 - 2\langle n\rangle] \\ &= \langle n^2\rangle - 2\langle n\rangle^2 - \langle n\rangle + \langle n_+n_-\rangle \\ &= \langle n_+n_-\rangle,\end{aligned} \tag{63}$$

where (59) has been used at the last step (and $\langle n_\pm\rangle = \langle n\rangle$ from the beginning). Thus the asymmetry of $\tilde\kappa_2$ in the two parameters arises from "interference" between two modes. The quantity is readily calculated by our method:

$$n_+n_- = \tfrac{1}{4}(O_N + O_T + O_O), \tag{64}$$

where

$$
\begin{aligned}
O_N &= G^\dagger G G_-^\dagger G_- + H^\dagger H H_-^\dagger H_- + G^\dagger G H_-^\dagger H_- + H^\dagger H G_-^\dagger G_- \,, \\
O_T &= G^\dagger G_-^\dagger H H_- + G G_- H^\dagger H_-^\dagger + G^\dagger G_- H_-^\dagger H + G_-^\dagger G H^\dagger H_- \,,
\end{aligned} \tag{65}
$$

and O_O comprises 8 terms with either three G operators and one H or vice versa. It is easy to see that O_O and the last two terms of O_T do not contribute to the expectation value of n_+n_- in $|0,0,0,0\}$. The calculation of $\frac{1}{4}\langle O_N \rangle$ is very similar to that of $\langle n^2 \rangle$ and results in the symmetric expression

$$
\frac{A^4 + 4A^2B^2 + B^4 + \frac{1}{2}(A^2 + B^2)(1 + A^2B^2)}{(1 - A^2)^2(1 - B^2)^2} \,. \tag{66}
$$

For $\frac{1}{4}\langle O_T \rangle$ one finally gets an asymmetric expression,

$$
\frac{\frac{1}{2}(A^2 - B^2)(1 - A^2B^2)}{(1 - A^2)^2(1 - B^2)^2} \,. \tag{67}
$$

Adding (66) and (67) and rearranging, one reproduces (62).

5.4 The quadratic moments for standing waves

The analog of $\langle n_+n_- \rangle$ for the standing modes is $\langle n_c n_s \rangle$, the expectation value being taken in $|0,0\}$ for the cosine and sine modes independently. Thus

$$
\langle n_c n_s \rangle = \langle n_c \rangle \langle n_s \rangle = \langle n \rangle^2 = \left[\frac{A^2 + B^2}{(1 - A^2)(1 - B^2)} \right]^2 . \tag{68}
$$

Clearly one must have

$$
\langle (n_c + n_s)^2 \rangle = \langle (n_+ + n_-)^2 \rangle, \tag{69}
$$

whence by (59) and (68) one has

$$
\begin{aligned}
\tfrac{1}{2}[\langle n_c^2 \rangle + \langle n_s^2 \rangle] &= -\langle n_c n_s \rangle + \langle n^2 \rangle + \langle n_+ n_- \rangle \\
&= \langle n \rangle^2 + \langle n \rangle + \langle n_+ n_- \rangle,
\end{aligned} \tag{70}
$$

which simplifies to the quantity (61) upon substitution from (53) and (62)–(63). Given that $\langle n_c^2 \rangle = \langle n_s^2 \rangle$, and that $\langle n_+ n_- \rangle$ is known, this argument is the easiest way to derive (61).

6 The generating function

6.1 The single-mode density matrix revisited

The matrix elements $\rho_{nn'} = \langle n|\rho|n'\rangle$ of (39) and (40) have been obtained by regarding the statistical operator ρ of (23) as referring to one mode of a two-mode system that is in the pure state $|0,0\}\{0,0|$. A different, and somewhat more direct, method of calculating $\rho_{nn'}$ first constructs the generating function

$$g(x,y) = \sum_{n,n'=0}^{\infty} \frac{x^n \langle n|\rho|n'\rangle y^{n'}}{\sqrt{n!\,n'!}} \tag{71}$$

and then expands it in powers of x and y. The bra and ket states that show up here as the summations over n and n' are recongnized as the well known coherent states (of Bargmann type), the eigenbras of $\beta^\dagger$ and eigenkets of β,

$$\sum_{n=0}^{\infty} \frac{x^n\langle n|}{\sqrt{n!}}(\beta^\dagger - x) = 0\,, \qquad (\beta - y)\sum_{n'=0}^{\infty} \frac{|n'\rangle y^{n'}}{\sqrt{n'!}} = 0\,. \tag{72}$$

These eigenvector equations are exploited upon writing ρ as a normally ordered function of $\beta^\dagger$ and β; that is, all $\beta^\dagger$s stand to the left of all βs. We begin with

$$\begin{aligned}\rho &= (1-e^{-\epsilon/T})e^{-(\epsilon/T)b^\dagger b} = (1-e^{-\epsilon/T})\exp\Bigl(-(1-e^{-\epsilon/T})b^\dagger; b\Bigr)\\ &= e^{\frac{1}{2}({\beta^\dagger}^2-\beta^2)\theta}(1-e^{-\epsilon/T})\exp\Bigl(-(1-e^{-\epsilon/T})\beta^\dagger;\beta\Bigr)e^{-\frac{1}{2}({\beta^\dagger}^2-\beta^2)\theta}\,,\end{aligned} \tag{73}$$

where

$$e^{X;Y} = \sum_{n=0}^{\infty}\frac{X^n Y^n}{n!} \tag{74}$$

denotes the basic ordered exponential function, for which the much used identity

$$(1-\lambda)^{b^\dagger b} = e^{-\lambda b^\dagger; b} \tag{75}$$

is a familiar application.

The $\beta^\dagger;\beta$-ordered version of ρ,

$$\rho = \sqrt{\lambda^2 - \mu^*\mu}\; e^{\frac{1}{2}\mu{\beta^\dagger}^2} e^{-\lambda\beta^\dagger;\beta} e^{\frac{1}{2}\mu^*\beta^2} \tag{76}$$

with

$$
\begin{aligned}
\lambda &= 1 - \frac{e^{-\epsilon/T}}{(\cosh\theta)^2 - e^{-2\epsilon/T}(\sinh\theta)^2}\,, \\
\mu = \mu^* &= (1 - e^{-2\epsilon/T})\frac{\sinh\theta\,\cosh\theta}{(\cosh\theta)^2 - e^{-2\epsilon/T}(\sinh\theta)^2}\,, \\
\sqrt{\lambda^2 - \mu^*\mu} &= \frac{1 - e^{-\epsilon/T}}{\sqrt{(\cosh\theta)^2 - e^{-2\epsilon/T}(\sinh\theta)^2}}\,,
\end{aligned}
\tag{77}
$$

can now be found by a variety of methods. It suffices to verify that it responds correctly to infinitesimal changes of θ.

Now, when using (76) in (71), the identities (72) permit the replacements $\beta^\dagger \to x$, $\beta \to y$, and then the summation is elementary,

$$
\sum_{n,n'=0}^{\infty} \frac{x^n \langle n|n'\rangle y^{n'}}{\sqrt{n!\,n'!}} = e^{xy}\,. \tag{78}
$$

We thus arrive at the explicit form of the generating function (71),

$$
g(x,y) = \sqrt{\lambda^2 - \mu^*\mu}\; e^{\frac{1}{2}\mu x^2} e^{(1-\lambda)xy} e^{\frac{1}{2}\mu^* y^2}\,. \tag{79}
$$

Such a two-dimensional Gaussian is a typical generating function for linear systems, since all time-transformation functions are of this form if the Heisenberg equations of motion are linear. A recent example is the parametric oscillator investigated by Rashid and Mahmood [29], who combine the Maclaurin series of the three exponential functions in (79) and get an answer where one summation is still to be done, somewhat like the situation in (40) above.

Here we wish to put a different approach on record. It exploits the well known fundamental generating function for Bessel functions of integer order (see 9.1.41 and 9.1.5 in [30]),

$$
e^{\frac{1}{2}z(t-1/t)} = \sum_{k=-\infty}^{\infty} t^k J_k(z) = \sum_{k=-\infty}^{\infty} t^k (-1)^{\frac{1}{2}(|k|-k)}(z)\,, \tag{80}
$$

and one of the generating functions for Gegenbauer polynomials of index $k + \frac{1}{2}$ (see 22.9.5 in [30]),

$$
e^u (z/2)^{-k} J_k(z) = \sum_{l=0}^{\infty} \frac{(2k)!}{k!\,(2k+l)!} (z^2 + u^2)^{\frac{1}{2}l} C_l^{(k+\frac{1}{2})}\left(u\middle/\sqrt{z^2+u^2}\right)\,, \tag{81}
$$

valid for $k \geq 0$. Jointly they amount to

$$e^{\frac{1}{2}z(t-1/t)+u} = \sum_{k=-\infty}^{\infty}\sum_{l=0}^{\infty} 2^{-|k|}(zt)^{\frac{1}{2}(|k|+k)}(-z/t)^{\frac{1}{2}(|k|-k)}\frac{(2|k|)!}{(|k|)!\,(2|k|+l)!} \times (z^2+u^2)^{\frac{1}{2}l} C_l^{(|k|+\frac{1}{2})}\left(u\Big/\sqrt{z^2+u^2}\right) . \qquad (82)$$

The left-hand side thereof turns into the product of exponentials in (79) if one puts

$$zt = \mu x^2 , \quad -z/t = \mu^* y^2 , \quad u = (1-\lambda)xy , \qquad (83)$$

so that

$$(z^2+u^2)^{\frac{1}{2}} = \sqrt{(1-\lambda)^2 - \mu^*\mu}\; xy , \qquad \frac{u}{\sqrt{z^2+u^2}} = \frac{1-\lambda}{\sqrt{(1-\lambda)^2-\mu^*\mu}} . \qquad (84)$$

Note that the latter, which is the argument of the Gegenbauer polynomial in (82), does not depend on x or y. All dependence on x and y is in the form of explicit powers.

Upon putting things together, we arrive at

$$\begin{aligned}\frac{g(x,y)}{\sqrt{\lambda^2-\mu^*\mu}} &= e^{\frac{1}{2}\mu x^2+(1-\lambda)xy+\frac{1}{2}\mu^* y^2} \\ &= \sum_{k=-\infty}^{\infty}\sum_{l=0}^{\infty} 2^{-|k|}\left(\mu x^2\right)^{\frac{1}{2}(|k|+k)}\left(\mu^* y^2\right)^{\frac{1}{2}(|k|-k)} \\ &\qquad \times \frac{(2|k|)!}{(|k|)!\,(2|k|+l)!}\left(\sqrt{(1-\lambda)^2-\mu^*\mu}\; xy\right)^l \\ &\qquad \times C_l^{(|k|+\frac{1}{2})}\left(\frac{1-\lambda}{\sqrt{(1-\lambda)^2-\mu^*\mu}}\right) , \end{aligned} \qquad (85)$$

where $n = |k|+k+l$ is the total power of x and $n' = |k|-k+l$ is that of y, their difference $n-n' = 2k$ and sum $n+n' = 2|k|+2l$ being even. We write

$$k = \frac{n-n'}{2} , \quad l = n_< = \min\{n,n'\} , \quad 2|k|+l = n_> = \max\{n,n'\} \qquad (86)$$

to present (85) as a sum over n and n'. This enables us to identify the matrix element $\langle n|\rho|n'\rangle = \rho_{nn'}$, with the outcome

$$\rho_{nn'} = \frac{(n_>-n_<)!}{(\frac{1}{2}(n_>-n_<))!}\left(\frac{n_<!}{n_>!}\right)^{\frac{1}{2}}\sqrt{\lambda^2-\mu^*\mu}$$

$$\times (\mu/2)^{\frac{1}{2}(n-n_<)}(\mu^*/2)^{\frac{1}{2}(n'-n_<)}\left((1-\lambda)^2-\mu^*\mu\right)^{\frac{1}{2}n_<}$$
$$\times C_{n_<}^{\left(\frac{1}{2}(n_>-n_<+1)\right)}\left(\frac{1-\lambda}{\sqrt{(1-\lambda)^2-\mu^*\mu}}\right) \tag{87}$$

if $n-n'$ is even, and $\rho_{nn'}=0$ if $n-n'$ is odd. In addition to the expressions of (77) we also meet here

$$(1-\lambda)^2-\mu^*\mu = \frac{e^{-2\epsilon/T}(\cosh\theta)^2-(\sinh\theta)^2}{(\cosh\theta)^2-e^{-2\epsilon/T}(\sinh\theta)^2}\,. \tag{88}$$

In fact, the result (87) is a bit too general for our purposes because we have the case of $\mu=\mu^*$, which simplifies matters somewhat. Expressed in terms of $A=\tanh\theta$ and $B=e^{-\epsilon/2T}$ we have, for $n-n'$ even,

$$\rho_{nn'} = \frac{(n_>-n_<)!}{(\frac{1}{2}(n_>-n_<))!}\left(\frac{n_<!}{n_>!}\right)^{\frac{1}{2}}\left(\frac{1-A^2}{1-A^2B^4}\right)^{\frac{1}{2}}(1-B^2)$$
$$\times\left(\frac{1}{2}\frac{A(1-B^4)}{1-A^2B^4}\right)^{\frac{1}{2}(n_>-n_<)}\left(\frac{B^4-A^2}{1-A^2B^4}\right)^{\frac{1}{2}n_<}$$
$$\times C_{n_<}^{\left(\frac{1}{2}(n_>-n_<+1)\right)}\left(\frac{(1-A^2)B^2}{\sqrt{(1-A^2B^4)(B^4-A^2)}}\right)\,. \tag{89}$$

6.2 Diagonal terms

The Gegenbauer polynomials of index $\frac{1}{2}$ are the Legendre polynomials, $C_n^{(\frac{1}{2})}=P_n$, so that the diagonal matrix elements are given by

$$\langle n|\rho|n\rangle = \rho_{nn} = \sqrt{\lambda^2-\mu^*\mu}\left((1-\lambda)^2-\mu^*\mu\right)^{\frac{1}{2}n}P_n\left(\frac{1-\lambda}{\sqrt{(1-\lambda)^2-\mu^*\mu}}\right). \tag{90}$$

Upon recalling the familiar generating function for Legendre polynomials,

$$\sum_{n=0}^{\infty} t^n P_n(x) = \frac{1}{\sqrt{1-2tx+t^2}}\,, \tag{91}$$

we obtain the corresponding generating function for ρ_{nn},

$$\sum_{n=0}^{\infty} e^{inu}\rho_{nn} = \left[\frac{\lambda^2-\mu^*\mu}{1-2(1-\lambda)e^{iu}+[(1-\lambda)^2-\mu^*\mu]e^{2iu}}\right]^{\frac{1}{2}}, \tag{92}$$

which one recognizes to be identical with (26) in [25] when the differences in notation are taken into account.

6.3 Comparison

The dependence of (89) on A and B, although complicated, is nicely consistent with the observations in Sec. 3. Only even powers of B appear; this is the symmetry of (40) under the interchange of Ω and Ψ. Similarly, the behavior under change of sign of Ω and Ψ is implemented by the factor $A^{(n_> - n_<)/2}$.

To establish direct contact between (89) and (40) we would need to expand

$$\rho_{nn'} \cosh\Omega \cosh\Psi = \rho_{nn'} \frac{1 - A^2B^2}{(1-A^2)(1-B^2)} \tag{93}$$

in powers of

$$\tanh\Omega = \frac{A+B}{1+AB} \quad \text{and} \quad \tanh\Psi = \frac{A-B}{1-AB}\,, \tag{94}$$

which looks like an unfairly difficult homework exercise. We have evaluated (89) and (40) numerically for a variety of values of the parameters, always finding excellent agreement.

Thus the method of the generating function has provided a formula, (89), that is simpler than the one provided by the method of the thermal Bogolubov transformation, (40). (Numerically, the latter involves more computation and requires truncation of an infinite series.) Nevertheless, the thermal Bogolubov method has given us an interesting and elegant way of looking at the problem, which illuminates its symmetries and may lead to further insights in the future. Furthermore, for observables of the sort studied in Sec. 5 the calculations based on the thermal pure state vectors, (29) or (45), appear to be competitive with the conventional methods.

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